

A NEW SIGNATURE OF QUANTUM PHASE TRANSITIONS FROM THE NUMERICAL RANGE

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ABSTRACT. Predicting quantum phase transitions by signatures in finite models has a long tradition. Here we consider the numerical range W of a finite dimensional one-parameter Hamiltonian, which is a planar projection of the convex set of density matrices. We propose the new geometrical signature of non-analytic points of class C^2 on the boundary of W . We prove that a discontinuity of a maximum-entropy inference map occurs at these points, a pattern which was earlier fostered as a signature of quantum phase transitions. More precisely, we reduce both phenomena to higher energy level crossings with the ground state energy.

1. INTRODUCTION

Quantum phase transitions are associated with the ground state of an infinite lattice system [55, 44] and are marked by non-analyticity of the ground state energy, energy level crossing with the ground state energy, or long-range correlation in the ground state. Quantum phase transitions have also been witnessed in terms of entropy of entanglement [66, 38], which quantifies entanglement, a form of correlations distinguished in quantum mechanics. Other interesting entropic correlation quantities in statistical mechanics are conditional mutual information and irreducible many-party correlation [14, 46, 35]. The latter is important also in classical statistical mechanics [47, 20] where no entanglement exists.

Quantum phase transitions in infinite lattice models are indicated by *signatures* in finite lattice models. Examples are the variation [3] or discontinuity [14] of a maximum-entropy inference map, the variation of many-party correlations [46], or the existence of ruled surfaces on three-dimensional projections of many-party states [15]. The present article discusses an arbitrary one-parameter Hamiltonian

$$H(g) := H_0 + g \cdot H_1$$

acting on the Hilbert space \mathbb{C}^d , $d \in \mathbb{N}$. We think of $H_0 \in M_d^h$ as an unperturbed Hamiltonian to which an external field $H_1 \in M_d^h$ is coupled by a real parameter g . Here M_d^h denotes the real subspace of hermitian matrices of the C^* -algebra M_d of d -by- d matrices with complex entries.

We discuss two signatures of a quantum phase transition associated with a planar convex set. The *numerical range* of $A = H_0 + i H_1$ is

$$W := W_A := \{\langle x | Ax \rangle : |x\rangle \in \mathbb{C}^d, \langle x | x \rangle = 1\}.$$

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We identify $\mathbb{C} \cong \mathbb{R}^2$. The numerical range $W \subset \mathbb{C}$ is convex, by a theorem of Toeplitz and Hausdorff [65, 28], compact, and non-empty. That is W is a *convex body*. The Hamiltonian H is recovered from the *real part* $H_0 = \operatorname{Re}(A)$ and *imaginary part* $H_1 = \operatorname{Im}(A)$ of A defined by

$$\operatorname{Re}(A) = \frac{1}{2}(A + A^*) \quad \text{and} \quad \operatorname{Im}(A) = \frac{1}{2i}(A - A^*).$$

Notice that for $\theta \in] -\frac{\pi}{2}, \frac{\pi}{2}[$ we have

$$\operatorname{Re}(e^{-i\theta}A) = \cos(\theta) \cdot H(\tan(\theta)).$$

For any $\theta \in \mathbb{R}$ we refer to the smallest eigenvalue $\lambda(\theta)$ of $\operatorname{Re}(e^{-i\theta}A)$ as the *ground state energy*, to the corresponding eigenspace as the *ground space*, and to any of its unit vectors as a *ground state* of $\operatorname{Re}(e^{-i\theta}A)$. For arbitrary unit vectors $|\phi\rangle \in \mathbb{C}^d$ and ground states $|\psi\rangle$ of $\operatorname{Re}(e^{-i\theta}A)$ we have [65]

$$(1.1) \quad \lambda(\theta) = \langle \psi | \operatorname{Re}(e^{-i\theta}A) | \psi \rangle \leq \langle \phi | \operatorname{Re}(e^{-i\theta}A) | \phi \rangle = \operatorname{Re} \langle e^{i\theta} | \langle \phi | A | \phi \rangle \rangle.$$

The usual scalar product of $z_1, z_2 \in \mathbb{C}$ being $\langle z_1, z_2 \rangle = \operatorname{Re} \langle z_1 | z_2 \rangle$, equation (1.1) shows that $\lambda(\theta)$ is the *support function* of W evaluated at $e^{i\theta}$ which by definition is the signed distance $\lambda(\theta) = \min_{z \in W} \langle z, e^{i\theta} \rangle$ of the origin from the supporting line of W with inner normal vector $e^{i\theta}$.

The ground state energy of $H(g)$ at $g \in \mathbb{R}$ is $\sqrt{1+g^2} \cdot \lambda(\arctan(g))$. Its maximal order of continuous differentiability at g is the same as that of λ at $\arctan(g)$ and the two functions are at corresponding points either both analytic or both non-analytic. We restrict forthcoming discussions to λ , which is well-known [53] to be piecewise analytic.

A new result of this article is that non-analytic points of class C^2 of ∂W , viewed as a submanifold¹ of \mathbb{C} , correspond to non-analytic points of class C^2 of the ground state energy λ , modulo 2π . The latter exist [41, 42], if $d \geq 4$. We prove their maximal order of continuous differentiability to be even and equal to that of ∂W . To this end we change viewpoints between ∂W as an *envelope* of supporting lines and ∂W as a *manifold*. For unit vectors $u \in \mathbb{C}$ where the supporting line of W with inner normal vector u meets W at a single point z of W , this point is the value $z = x_W(u)$ of the reverse spherical image map [57], which we call *reverse Gauss map* x_W . The points in the image of x_W are exposed point of W . Under suitable restrictions, x_W is inverse to the *Gauss map* which sends smooth boundary points to normal vectors. That ∂W is an envelope of supporting lines means that x_W is the gradient of the positive homogeneous extension of the support function λ . Parametrized by x_W , the manifold ∂W would seem to be of a lower differentiability class than λ . This problem is overcome [57] in a detour through the dual convex body of W . Thereby it is essential that W has strictly positive radii of curvature at smooth boundary points [19, 29, 21, 61, 56, 27].

Returning to signatures of quantum phase transitions, the pioneering work [3] shows that critical phenomena in fermion systems correspond to strong variations of a maximum-entropy inference map (*MaxEnt map*) under expectation value constraints of carefully chosen observables. By definition, the MaxEnt map sends an n -tuple of real numbers to the quantum state which maximizes the von Neumann

¹For $k \geq 1$, a C^k -submanifold M of \mathbb{C} is a subset $M \subset \mathbb{C}$ such that for each point p of M there is a (real) C^k -diffeomorphism $g : U \rightarrow V$ from an open neighborhood U of p in \mathbb{C} to an open neighborhood V of 0 in \mathbb{R}^2 such that $g(M \cap U)$ lies in the x_1 -axis of \mathbb{R}^2 . The subset M is an *analytic submanifold* of \mathbb{C} , if g can be chosen to be an analytic diffeomorphism.

entropy among all states for which the expectation values of the observables match the tuple [32]. The values of the MaxEnt map are also known as thermal states because they describe quantum systems in thermal equilibrium [4, 74].

A pronounced variation of a MaxEnt map is its discontinuity, which was proposed as a signature of quantum phase transitions [14] in the above setting of a one-parameter Hamiltonian. The domain of the MaxEnt map is W_A for the observables $\operatorname{Re}(A)$ and $\operatorname{Im}(A)$. Indeed, let \mathcal{M}_d denote the *state space* [2] of M_d , which is the set of positive semi-definite matrices of trace one in M_d , also known as *density matrices*. The numerical range is the projection $W_A = \{\operatorname{tr}(\rho A) : \rho \in \mathcal{M}_d\}$ of the state space [7], and represents the expectation values [6] of $\operatorname{Re}(A)$ and $\operatorname{Im}(A)$. Discontinuity points of this MaxEnt map exist [72] on W for $d \geq 3$ and are non-removable, as shown in Theorem 2d of [73]. We give a new proof that points of discontinuity correspond to crossing of class C^2 between a higher energy level and the ground state energy λ , modulo 2π . The work [70] derives this result from [41] using functional analysis. Our new proof uses two extensions of the reverse Gauss map x_W to parametrize the extreme points of W , where the discontinuities are located. Roughly speaking, a normal vector $e^{i\theta}$ corresponds to a Hamiltonian $\operatorname{Re}(e^{-i\theta}A)$ whose ground space specifies the value of the MaxEnt map at the exposed point $x_W(e^{i\theta})$.

Three remarks are in order. First, we do not suppose that the energy operators $H_0 = \operatorname{Re}(A)$ and $H_1 = \operatorname{Im}(A)$ or their expectation values are measurable. Rather, our results confirm that the geometry of W and the continuity of the MaxEnt map $W \rightarrow \mathcal{M}_d$ capture relevant information about the ground state energy λ , even when the expectation values of H_0 and H_1 are unknown or inaccessible [13, 12].

Second, our analysis includes one-sided level crossings with a non-differentiable λ and discontinuity points of the MaxEnt map at non-exposed points of W . Non-differentiability of λ at θ means that the supporting line with inner normal vector $e^{i\theta}$ intersects W at a flat portion of the boundary. We point out that for commutative operators $H_0H_1 = H_1H_0$ the function λ is piecewise harmonic and has no level crossings of class C^2 , while W is a polytope and the MaxEnt map is continuous [69].

Third, W plays a broader role in physics, for example in understanding entanglement [52], and has a beautiful geometry including algebraic curves [36, 17] or critical values [33, 34]. Another theory affiliated to W is positivity in C^* -algebras, because W is a planar projection of the state space \mathcal{M}_d . We hope our results are useful to understand more general projections of state spaces, in particular reduced density matrices (quantum marginals) which appear in state representation problems [50], and in the field of quantum phase transitions as marginals represent, similarly to (1.1), the ground state energy of local Hamiltonians [25]. For example, quantum phase transitions were identified through ruled surfaces on three-dimensional projections of several classes of states in Landau's symmetry-breaking theory [75] and the theory of topological phases² [15].

Section 2 introduces convex geometry and radii of curvature of W . Section 3 customizes differential geometry of planar convex sets. Section 4 applies them to W and adds a discussion of differentiability orders. Section 5 studies the continuity of the MaxEnt map and of a multi-valued map known from operator theory.

²We remark that topological phases are characterized by topological entanglement entropy [37, 43], see for example [31], but they were also described in terms of the variation of entropic correlation quantities [14, 46, 35].

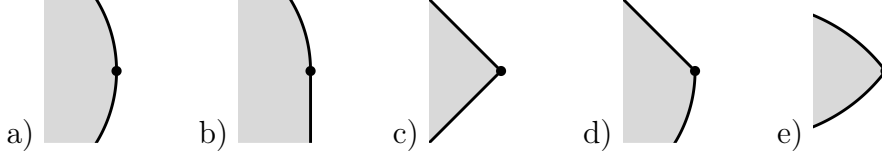


FIGURE 1. Extreme points of planar two-dimensional convex bodies. Regular extreme points: a) regular exposed point, b) non-exposed point. Corner points incident with c) two, d) one, or e) no facet(s).

2. DONOGHUE'S THEOREM AND RELATIVES

The numerical range W has a special smoothness as it is locally a triangle at non-smooth boundary points. The boundary ∂W is also featured in respect to curvature because the one-sided radii of curvature exist and are strictly positive at all smooth boundary points. Finite radii of curvature exist at all smooth exposed points.

Let $K \subset \mathbb{R}^n$ be a convex subset. To discuss smoothness of ∂K we consider \mathbb{R}^n as a Euclidean vector space with the standard scalar product $\langle \cdot, \cdot \rangle$. An *inner normal vector* of K at $x \in K$ is a vector $u \in \mathbb{R}^n$ which has no obtuse angle with the vector from x to any point of K , that is

$$\langle y - x, u \rangle \geq 0 \quad \forall y \in K.$$

The set of inner normal vectors of K at x is a closed convex cone, called *normal cone* of K at x . This cone is non-zero if and only if x is a boundary point of K . In that case x is a *regular*, or *smooth*, boundary point of K , if K has a unique inner unit normal vector at x . Otherwise x is a *singular*, or *non-smooth*, boundary point of K . We call x *corner point* of K if the normal cone of K at x is n -dimensional.

There are several notion of flatness of the boundary ∂K . A *face* of K is a convex subset $F \subset K$ which contains every closed segment of K whose relative interior³ it intersects. If a singleton $\{x\}$ is a face of K then x is called *extreme point* of K . Examples of faces of K are *exposed faces* which are defined as subsets of minimizers of a linear functional on K . The empty set is an exposed face of K by convention. A face which is no exposed face is called *non-exposed face*. If a singleton $\{x\}$ is a (non-) exposed face of K then x is called (non-) *exposed point* of K . A face of K of codimension one in K is called a *facet* of K . All facets of K are exposed faces of K . Further, the family of relative interiors of faces of K is a partition of K .

In the remainder of this section we assume $K \subset \mathbb{R}^2$ and $\dim(K) = 2$. We denote the set of regular boundary points, regular extreme points, and regular exposed points of K , respectively, by

$$(2.1) \quad \text{reg}(K) \supset \text{reg ext}(K) \supset \text{reg exp}(K).$$

The mentioned partition applied to regular boundary points shows that $z \in K$ is a regular extreme point of K if and only if z is a regular boundary point which does not lie in the relative interior of a facet of K . This is the equivalence between (1) and (2) of Lemma 2.2.

A classification of extreme points of K , in terms of smoothness and flatness, is easy to state. Every singular extreme point of K is a corner point and hence an exposed point. Every regular extreme point z of K lies on at most one facet of K . Otherwise

³The *relative interior* of a subset M of \mathbb{R}^n is the interior of M with respect to the topology of the affine hull of M .

	exposed	regular	# incident facets
regular exposed point	yes	yes	0
non-exposed point	no	yes	1
corner point	yes	no	2

TABLE 1. Extreme points of two-dimensional numerical ranges. The cases a)–c) of Figure 1 are possible, but d) and e) are inconsistent with Theorem 2.1.

z would be an intersection of two facets. The antitone lattice isomorphism between exposed faces and normal cones [68] then shows that z is a singular boundary point, which is a contradiction. Since $\dim(K) = 2$ holds, z is an exposed point if z lies on no facet. Otherwise, by definition, the regular extreme point z is a non-exposed point. Figure 1 shows all possible cases, compactness of K is assumed to count incident facets.

If K is the numerical range $W = W_A$ of a matrix $A \in M_d$, then a theorem by Donoghue [19] affirms that every corner point z of W is an eigenvalue of A . In particular, W has at most finitely many corner points. The reason is that no non-degenerate ellipse included in W can pass through z . A closer look at Donoghue's proof shows that z is indeed a *normal splitting eigenvalue* of A , that is there is a non-zero $x \in \mathbb{C}^d$ such that $Ax = zx$ and $A^*x = \bar{z}x$ hold. This gives an orthogonal direct sum decomposition $A = (z) \oplus B$ where $B \in M_{d-1}$ (we ignore the unitary conjugation which brings A into this form). Since W_A is the convex hull of z and W_B , either $z \notin W_B$ or an analogue decomposition applies to B . Inductively, W is the convex hull of z and W_C for some matrix C with $z \notin W_C$. Thus z is incident with two facets of W . This proves the following statement.

Theorem 2.1. *Let $\dim(W) = 2$ and let z be a corner point of W . Then z is the intersection of two facets of W .*

See Lemma 6.1 of [54] for a similar proof of Theorem 2.1. Table 1 lists the resulting classification of extreme points.

Let us characterize regular extreme points. A point $z \in K$ is a *round boundary point* of K if $z \in \partial K$ and for all $\epsilon > 0$ at least one of the one-sided ϵ -neighborhoods of z in ∂K is not a line segment [18, 41].

Lemma 2.2. *Let $K \subset \mathbb{R}^2$ be a compact convex subset, $\dim(K) = 2$, and let $z \in \partial K$. Then we have (1) \iff (2) \implies (3) \iff (4). If $K = W$ then also (3) \implies (2).*

- (1) $z \in \text{reg ext}(K)$,
- (2) z is no corner point of K and no relative interior point of a facet of K ,
- (3) z is an extreme point of K which is incident with at most one facet of K ,
- (4) z is a round boundary point of K .

Proof: (1) \iff (2) is proved in the paragraph of (2.1). For (1) \implies (3) we refer to one paragraph after (2.1), see also Figure 1. We prove (3) \implies (4) by contradiction: If z is an extreme point whose two one-sided neighborhoods are segments then these segments can be extended to two facets. (4) \implies (3) is easy to prove indirectly. If $K = W$ is the numerical range then (3) \implies (1) follows indirectly because corner

points lie on two facets, see the second paragraph above this lemma. \square

The statement (1) respectively (2) of Lemma 2.2 is the definition of *round boundary point* in [40, 54, 45], respectively [62]. A stronger definition than round boundary point appears in [41]: A point $z \in K$ is a *fully round boundary point* of K , if $z \in \partial K$ and for all $\epsilon > 0$ both one-sided ϵ -neighborhoods of z in ∂K are no line segments.

Lemma 2.3. *Let $K \subset \mathbb{R}^2$ be a compact convex subset, $\dim(K) = 2$, and let $z \in \partial K$. Then we have $(1) \iff (2) \implies (3) \iff (4)$. If $K = W$ then also $(3) \implies (2)$.*

- (1) $z \in \text{reg exp}(K)$,
- (2) z is no corner point of K , no non-exposed point of K , and no relative interior point of a facet of K ,
- (3) z is an extreme point of K which is not incident with any facet of K ,
- (4) z is a fully round boundary point of K .

Proof: The proof is analogous to the proof of Lemma 2.2. \square

Outside of corner points, the geometry of ∂W is characterized by its curvature. Let $z \in \text{reg}(K)$. Choose the cartesian coordinate system of \mathbb{R}^2 such that $z = (0, 0)$ and $K \subset \{(\xi, \eta) \in \mathbb{R} : \eta \geq 0\}$ (orthogonal coordinates in standard orientation). Then there is $\epsilon > 0$ and a convex function $f :]-\epsilon, \epsilon[\rightarrow \mathbb{R}$ such that $\xi \mapsto (\xi, f(\xi))$ parametrizes ∂K locally around z . Recall that $f'(0) = 0$ holds, for example see Section 2 of [10] or Theorem 1.5.4 of [57].

Using the notation from the preceding paragraph, we define the *counterclockwise* respectively *clockwise curvature* of ∂K at z by

$$(2.2) \quad \kappa_+(z) := \lim_{\xi \searrow 0} \frac{2f(\xi)}{\xi^2} \quad \text{respectively} \quad \kappa_-(z) := \lim_{\xi \nearrow 0} \frac{2f(\xi)}{\xi^2},$$

if the limit exists. The one-sided *radii of curvature* of ∂K at z are $\rho_{\pm}(z) := 1/\kappa_{\pm}(z)$. To connect to the literature, we define the *upper* respectively *lower curvature* of ∂K at z to be

$$(2.3) \quad \kappa_s(z) := \limsup_{\xi \rightarrow 0} \frac{2f(\xi)}{\xi^2} \quad \text{respectively} \quad \kappa_i(z) := \liminf_{\xi \rightarrow 0} \frac{2f(\xi)}{\xi^2}.$$

If $\kappa_s(z) = \kappa_i(z)$ then $\kappa(z) := \kappa_s(z)$ is the *curvature* and $\rho(z) := 1/\kappa(z)$ the *radius of curvature* of ∂K at z , including possible values of $\{0, +\infty\}$. A formula for $\rho(z)$ is known [22].

Recall that if f is twice differentiable at the origin then $\kappa(z) = f''(0)$ holds because (2.2) denotes the second right and left *de la Vallée-Poussin* derivatives of f at the origin, see Section 2 of [10]. If f is C^2 at the origin and $f''(0) > 0$ then $\rho(z) = 1/f''(0)$ is the radius of the osculating circle of ∂K at z , see for example [63].

It may happen that $\kappa(z) = \infty$, for example when $1 < \alpha < 2$ and $f(\xi) = \xi^\alpha$ holds in a neighborhood of $\xi = 0$, but this is impossible for $K = W$. Indeed, it was conjectured [29] that for a bounded operator on a Hilbert space all regular boundary points of the numerical range with infinite lower curvature belong to the essential spectrum of that operator.

This conjecture was proved independently in [21, 56, 61]. It was shown in [27] that ideas of [19, 61] yield a somewhat stronger result, which we cite in the form of Theorem 2.4, and for which we give a simple proof in finite dimensions.

Theorem 2.4 (Farid, Salinas and Velasco, I. M. S., and Hansmann). *Let $z \in \partial W$ be a regular boundary point. Then $\kappa_s(z) < \infty$.*

Proof: (Indirectly) It was pointed out in [27] that no non-degenerate ellipse included in W can pass through $z \in \text{reg}(W)$, if $\kappa_s(z) = \infty$, and that therefore, following the reasoning of [19], z is an eigenvalue of A . As stressed in the above proof of Theorem 2.1, z is in fact a normal splitting eigenvalue of A and a corner point of W . \square

3. DIFFERENTIAL GEOMETRY OF PLANAR CONVEX BODIES

We study two maps $x_{K,\pm}$ from the unit circle S^1 to the extreme points of a planar convex body K . If the values of $x_{K,\pm}$ agree at a normal vector then they agree with the *reverse Gauss map* x_K . Otherwise x_K is undefined and $x_{K,\pm}$ describe pairs of distinct extreme points of boundary segments. The image of x_K intersected with the regular boundary points is the set of regular exposed points $\text{reg exp}(K)$ whose differential geometry will be the focus of this section, along with limit points of the set $\text{reg exp}(K)$. Since the differentiability order of x_K is too small for our purposes we will also study a dual convex body K^* .

Let $K \subset \mathbb{R}^2$ be a convex body. The *support function* of K is

$$\mathbf{h}_K : \mathbb{R}^2 \rightarrow \mathbb{R}, \quad u \mapsto \min_{x \in K} \langle x, u \rangle.$$

The function \mathbf{h}_K is concave, continuous, and positively homogenous [57]. Non-empty exposed faces of K are parametrized in terms of their inner normal vectors by

$$F_K : \mathbb{R}^2 \rightarrow 2^K, \quad u \mapsto \underset{x \in K}{\text{argmin}} \langle x, u \rangle,$$

where 2^K denotes the set of subsets of K . If u is a unit vector then $F_K(u)$ is a singleton or a closed segment and we can denote its extreme point(s) by $x_{K,+}(u)$ and $x_{K,-}(u)$. Formally, we define two maps $x_{K,+}$ and $x_{K,-}$ by

$$x_{K,\pm} : S^1 \rightarrow \partial K, \quad u \mapsto u \cdot [\mathbf{h}_K(u) \pm i \mathbf{h}_{F_K(u)}(\pm i u)].$$

The union of the images of $x_{K,\pm}$ is the set of extreme points of K . Indeed, $x_{K,\pm}(u)$ is an extreme point of K since it is an extreme point of $F_K(u)$. Conversely, every non-exposed point of K is an exposed point of a facet of K , see Figure 1 b), and see [62] for more details⁴. For all extreme points z of K and unit vectors $u \in S^1$, a general property of normal vectors and exposed faces [68], applied to the exposed face $F_K(u)$, proves that

$$(3.1) \quad z = x_{K,\pm}(u) \iff u \text{ is an inner normal vector of } K \text{ at } z.$$

Thereby $z = x_{K,\pm}(u)$ stands for $z = x_{K,+}(u)$ or $z = x_{K,-}(u)$, but not necessarily for both. In the following the meaning of the \pm -symbol will be clear from the context.

A unit vector $u \in S^1$ is a *regular normal vector* [57] of K if $x_{K,+}(u) = x_{K,-}(u)$ holds, that is, if $F_K(u)$ is a singleton. Otherwise we call u *singular normal vector*. Let $\text{regn}(K)$ denote the set of regular normal vectors of K , and let

$$\Xi_K := \{\theta \in \mathbb{R} : e^{i\theta} \in \text{regn}(K)\}$$

⁴The idea of viewing non-exposed points as exposed points of facets is a special case of the conception of *poonem* [24].

$$\begin{array}{ccccc}
\text{reg exp}(K) & \xrightleftharpoons{\quad} & R_K & \xleftarrow{\quad} & \Xi_K^R \\
\downarrow & & \downarrow & & \downarrow \\
\text{reg}(K) & & \text{regn}(K) & \xleftarrow{\quad} & \Xi_K \\
\downarrow & \swarrow x_K & \downarrow & \searrow u_K & \downarrow \\
\partial K & & S^1 & \xleftarrow{\theta \mapsto e^{i\theta}} & \mathbb{R}
\end{array}$$

FIGURE 2. Commutative diagram for the Gauss map u_K and reverse Gauss map x_K of a planar convex body K with angular parametrizations. Hooked arrows denote embeddings.

be its angular representation. The *reverse Gauss map* is defined by

$$x_K : \text{regn}(K) \rightarrow \partial K, \quad \{x_K(u)\} = F_K(u).$$

The *Gauss map* is the function

$$u_K : \text{reg}(K) \rightarrow S^1$$

such that $u_K(x)$ is the unique inner unit normal vector of K at $x \in \text{reg}(K)$.

Notice that the image of x_K is the set of exposed points of K . Its intersection with the domain of u_K is the set $\text{reg exp}(K)$ of regular exposed points of K . Both the Gauss map u_K and the reverse Gauss map x_K are continuous, see for example Section 2.2 of [57]. The restriction of u_K to $\text{reg exp}(K)$ is a homeomorphism onto

$$R_K := \{u_K(x) : x \in \text{reg exp}(K)\},$$

whose inverse homeomorphism is the restriction of x_K . Let

$$\Xi_K^R := \{\theta \in \mathbb{R} : e^{i\theta} \in R_K\}$$

be the angular representation of inner unit normal vectors at regular exposed points. A diagram is shown in Figure 2.

Although \mathbf{h}_K may not be differentiable, its directional derivatives do exist. The *directional derivative* of $f : \mathbb{R}^k \rightarrow \mathbb{R}$ at $u \in \mathbb{R}^k$ in the direction of $v \in \mathbb{R}^k$ is

$$f'(u; v) := \lim_{t \searrow 0} [f(u + tv) - f(u)]/t,$$

if the limit exists. For $u, v \in \mathbb{R}^2$ we have $\mathbf{h}_{F_K(u)}(v) = \mathbf{h}'_K(u; v)$, see for example Theorem 1.7.2 of [57] or Section 16 of [9]. In particular,

$$\mathbf{h}_{F_K(u)}(\pm i u) = \mathbf{h}'_K(u; \pm i u), \quad u \in S^1,$$

which shows

$$(3.2) \quad x_{K,\pm}(u) = u \cdot [\mathbf{h}_K(u) \pm i \mathbf{h}'_K(u; \pm i u)], \quad u \in S^1.$$

Let $h_K(\theta) := \mathbf{h}_K(e^{i\theta})$, $\theta \in \mathbb{R}$. An easy calculation, see for example Lemma 2.2 of [62], shows

$$(3.3) \quad h'_K(\theta; \pm 1) = \mathbf{h}'_K(e^{i\theta}; \pm i e^{i\theta}), \quad \theta \in \mathbb{R}.$$

One obtains

$$(3.4) \quad x_{K,\pm}(e^{i\theta}) = e^{i\theta} \cdot [h_K(\theta) \pm i h'_K(\theta; \pm 1)]$$

from the preceding equations (3.2) and (3.3).

First order differentiability of \mathbf{h}_K is perfectly understood. Since \mathbf{h}_K is positively homogeneous, we have for $r > 0$ and $\theta \in \mathbb{R}$

$$\frac{\partial}{\partial r} \mathbf{h}_K(re^{i\theta}) = \mathbf{h}_K(e^{i\theta}) = h_K(\theta).$$

For all $\theta \in \Xi_K$ we get from (3.3)

$$\frac{\partial}{\partial \theta} \mathbf{h}_K(re^{i\theta}) = r \frac{\partial}{\partial \theta} \mathbf{h}_K(e^{i\theta}) = rh'_K(\theta).$$

Hence, \mathbf{h}_K is differentiable on open subsets of $\{ru : r > 0, u \in \text{regn}(K)\}$ and the gradient is

$$(3.5) \quad \nabla \mathbf{h}_K(re^{i\theta}) = e^{i\theta}[h_K(\theta) + i h'_K(\theta)], \quad r > 0, \theta \in \Xi_K.$$

The equations (3.4) and (3.5) show

$$(3.6) \quad x_K(e^{i\theta}) = e^{i\theta}[h_K(\theta) + i h'_K(\theta)] = \nabla \mathbf{h}_K(e^{i\theta}), \quad \theta \in \Xi_K.$$

Since x_K is continuous, \mathbf{h}_K is a C^1 -map on open subsets of $\{ru : r > 0, u \in \text{regn}(K)\}$, and h_K is a C^1 -map on open subsets of Ξ_K .

Second derivatives of \mathbf{h}_K are needed to address first derivatives of x_K and radii of curvature of ∂W . Let $\Xi_K^{(2)} \subset \Xi_K$ denote the largest open set in \mathbb{R} on which h_K is twice continuously differentiable. It follows from (3.5) that for all $r > 0$ and $\theta \in \Xi_K^{(2)}$ the Jacobian of $\nabla \mathbf{h}_K$ at $re^{i\theta}$ with respect to the orthonormal basis $\{e^{i\theta}, i e^{i\theta}\}$ is

$$\nabla \mathbf{h}_K(re^{i\theta}) = \frac{1}{r} \begin{pmatrix} 0 & 0 \\ 0 & h_K(\theta) + h''_K(\theta) \end{pmatrix}.$$

This shows that \mathbf{h}_K is a C^2 -map on the open set $\{re^{i\theta} : r > 0, \theta \in \Xi_K^{(2)}\}$. Since \mathbf{h}_K is concave, the above matrix is negative semi-definite. This shows

$$(3.7) \quad h_K(\theta) + h''_K(\theta) \leq 0, \quad \theta \in \Xi_K^{(2)}.$$

Moreover, (3.6) shows that x_K is a C^1 -map on $\{e^{i\theta} : \theta \in \Xi_K^{(2)}\} \subset S^1$, whose differential

$$(3.8) \quad (dx_K)_{e^{i\theta}}(i e^{i\theta}) = i e^{i\theta} \cdot [h_K(\theta) + h''_K(\theta)], \quad \theta \in \Xi_K^{(2)},$$

is defined on the tangent space of S^1 at $e^{i\theta}$. The differential $(dx_K)_{e^{i\theta}}$ is known as the *reverse Weingarten map* [57]. Its eigenvalue is $h_K(\theta) + h''_K(\theta)$. The non-negative number $-h_K(\theta) - h''_K(\theta)$ is the radius of curvature of ∂K at $x_K(e^{i\theta})$, see for example Section 39 of [9]. More generally, the one-sided radii of curvature, defined in the paragraph of (2.2), are as follows.

Lemma 3.1 (Radii of curvature). *Let z be a $\text{reg}(K)$ and let $] \varphi_1, \varphi_2[\subset \Xi_K^{(2)}$ be an open interval on which $h_K + h''_K$ is strictly negative. If $z = \lim_{\theta \searrow \varphi_1} x_K(e^{i\theta})$ respectively $z = \lim_{\theta \nearrow \varphi_2} x_K(e^{i\theta})$ then*

$$\rho_+(z) = - \lim_{\theta \searrow \varphi_1} [h_K(\theta) + h''_K(\theta)], \quad \text{respectively} \quad \rho_-(z) = - \lim_{\theta \nearrow \varphi_2} [h_K(\theta) + h''_K(\theta)].$$

Proof: Without loss of generality let $\varphi_1 = 0$ and assume $z = \lim_{\theta \searrow 0} x_K(e^{i\theta})$. Notice that $x_K(1)$ lies on the vertical supporting line to the left of K and that the curve $x_K(e^{i\theta})$, $\theta \in]0, \varphi_2[$, parametrizes an arc of ∂K which extends counterclockwise from z along ∂K . The latter follows also from by (3.17). The coordinates of $x_K(e^{i\theta})$, introduced in the paragraph preceding (2.2), are

$$(\xi, \eta) = [-\text{Im } v(\theta), \text{Re } v(\theta)],$$

where $v(\theta) := x_K(e^{i\theta}) - z$. We recall from (3.8) that $v'(\theta) = ie^{i\theta}f(\theta)$ holds, where we abbreviate $f(\theta) := h_K(\theta) + h_K''(\theta)$. By the assumption $f(\theta) < 0$ we have

$$\operatorname{Re}(v(\theta))' = \operatorname{Re}(v'(\theta)) = -\operatorname{Im}(e^{i\theta})f(\theta) = -\sin(\theta)f(\theta) \neq 0.$$

Twice applying l'Hôpital's rule then gives

$$\rho_+(z) = \lim_{\theta \searrow 0} \frac{\operatorname{Im}(v(\theta))^2}{2 \operatorname{Re}(v(\theta))} = \lim_{\theta \searrow 0} \frac{\operatorname{Im}(v(\theta)) \cos(\theta)}{-\sin(\theta)} = -\lim_{\theta \searrow 0} f(\theta).$$

The proof for the clockwise radius of curvature is analogous. \square

Our next aim is to relate the differentiability of $\operatorname{reg} \exp(K) \subset \partial K$ as a submanifold of \mathbb{C} and the differentiability of h_K as a function. Our proof is a generalization of two passages from pages 115 and 120 in Section 2.5 of [57], where the analogous statements are proved globally. Notice from Lemma 3.1 that radii of curvature depend on the support function. Thus the statements of Lemma 3.2 and Theorem 3.3 distinguish conceptually between ∂K as a manifold and h_K as a function.

Lemma 3.2. *Let $z \in \operatorname{reg} \exp(K)$ and $\theta \in \Xi_K^R$ be such that $z = x_K(e^{i\theta})$, and let $k \geq 2$. If $\operatorname{reg} \exp(K)$ is locally at z a C^k -submanifold of \mathbb{C} and u_K is locally at z a C^{k-1} -diffeomorphism then h_K is locally at θ of class C^k and the radius of curvature of ∂K is finite and strictly positive at z .*

Proof: Let $M \subset \operatorname{reg} \exp(K)$ be a C^k -submanifold of \mathbb{C} such that $U := u_K(M)$ is an open arc segment of S^1 and let $z \in M$. The support function is

$$(3.9) \quad \mathbf{h}_K(u) = \langle x_K(u), u \rangle, \quad u \in U,$$

because $U \subset \operatorname{reg} n(K)$. By assumption, u_K is a C^{k-1} -diffeomorphism on M . Hence the inverse x_K , defined on U , is of class C^{k-1} . Now (3.9) shows that \mathbf{h}_K is of class C^{k-1} on $\{ru : r > 0, u \in U\}$. In particular \mathbf{h}_K is differentiable, so (3.6) proves

$$\nabla \mathbf{h}_K(u) = x_K(u), \quad u \in U.$$

This shows that \mathbf{h}_K is of class C^k in a neighborhood of $u_K(z)$, so that h_K is of class C^k in a neighborhood of θ . The eigenvalue of the differential $(dx_K)_{e^{i\theta}} \in U$ is $h_K(\theta) + h_K''(\theta) < 0$ by (3.8) and (3.7), since x_K is a diffeomorphism on U . Lemma 3.1 shows that the radius of curvature of M at z is $-h_K(\theta) - h_K''(\theta) > 0$. \square

To prove a converse of Lemma 3.2, let us assume without loss of generality that $0 \in \mathbb{C}$ is an interior point of K . This is justified because the support function transforms under a translation by a vector $v \in \mathbb{C}$ into $\mathbf{h}_{K+v} = \mathbf{h}_K + \mathbf{h}_v$ where \mathbf{h}_v is linear. The *dual* of K ,

$$K^* := \{u \in \mathbb{C} : 1 + \langle u, z \rangle \geq 0, z \in K\},$$

is a convex body with 0 in its interior, and $(K^*)^* = K$ holds. For every convex subset $F \subset K$ the set

$$\mathcal{C}_K(F) := \{u \in K^* : 1 + \langle u, z \rangle = 0, z \in F\}$$

is an exposed face of K^* . We call $\mathcal{C}_K(F)$ the *dual face* of F . Let us also define the *normal cone* of K at F by

$$N_K(F) := \{u \in \mathbb{C} : \langle u, y - z \rangle \geq 0, y \in K, z \in F\}.$$

We write $N_K(z) := N_K(\{z\})$ and $\mathcal{C}_K(z) := \mathcal{C}_K(\{z\})$ for $z \in K$. The *positive hull* of a non-empty subset $U \subset \mathbb{C}$ is $\text{pos}(U) := \{ru : u \in U, r \geq 0\}$ while $\text{pos}(\emptyset) := \{0\}$ by convention.

We use a single property of the dual convex body K^* , namely that the conjugate face map sends a regular exposed point z of K to a regular exposed point of K^* by scaling the inner unit normal vector u of K at z with the radius of K^* in the direction of u . To begin with, we recall that $\mathcal{C}_{K^*}[\mathcal{C}_K(F)]$ is the smallest exposed face of K containing a convex subset $F \subset K$. Further, we have

$$(3.10) \quad N_K(F) = \text{pos}[\mathcal{C}_K(F)],$$

see for example Lemma 2.2.3 of [57]. For regular boundary points z of K the normal cone $N_K(z)$ is a ray and $\mathcal{C}_K(z)$ is a singleton. Then $\mathcal{C}_K(z) = x_{K^*}(z/|z|)$ follows from an easy calculation, and (3.10) shows

$$u_K(z) = x_{K^*}\left(\frac{z}{|z|}\right) / |x_{K^*}\left(\frac{z}{|z|}\right)|, \quad z \in \text{reg}(K).$$

Replacing K with the dual convex body K^* gives

$$(3.11) \quad u_{K^*}(u) = \frac{x_K(u/|u|)}{|x_K(u/|u|)|}, \quad u \in \text{reg}(K^*).$$

For exposed points $z \in K$, equation (3.10) proves $N_{K^*}(\mathcal{C}_K(z)) = \text{pos}(z)$, because of $\mathcal{C}_{K^*}[\mathcal{C}_K(z)] = z$. This shows that \mathcal{C}_K restricts to a bijection

$$(3.12) \quad \text{reg exp}(K) \rightarrow \text{reg exp}(K^*), \quad z \mapsto x_{K^*}(z/|z|) = u_K(z) \cdot \mathbf{r}_{K^*}(u_K(z)),$$

except for the equality on the right-hand side. To see this equality we use the *radial function* $\mathbf{r}_K : \mathbb{R}^2 \setminus \{0\} \rightarrow \mathbb{R}$, $u \mapsto \max\{r \geq 0 : r \cdot u \in K\}$, which is the multiplicative inverse of \mathbf{h}_{K^*} [57]. Replacing K and K^* , this means

$$(3.13) \quad \mathbf{r}_{K^*}(u) = -\mathbf{h}_K(u)^{-1}, \quad u \in \mathbb{R}^2 \setminus \{0\}.$$

The equality in (3.12) follows from (3.10) and (3.13).

Theorem 3.3. *Let $z \in \text{reg exp}(K)$ and $\theta \in \Xi_K^R$ be such that $z = x_K(e^{i\theta})$, and let $k \geq 2$. Then $\text{reg exp}(K)$ is locally at z a C^k -submanifold of \mathbb{C} and u_K is locally at z a C^{k-1} -diffeomorphism if and only if h_K is locally at θ of class C^k and the radius of curvature of ∂K is finite and strictly positive at z .*

Proof: One direction is proved in Lemma 3.2.

Conversely, let h_K be locally at θ of class C^k and let the radius of curvature of ∂K at $z = x_K(e^{i\theta})$ be strictly positive. We assume that 0 is an interior point of K and show that $\text{reg exp}(K^*)$ is locally at $\mathcal{C}_K(z)$ a C^k -submanifold of \mathbb{C} . The map $\mathcal{C}_K \circ x_K : R_K \rightarrow \text{reg exp}(K^*)$ to the dual convex body has by (3.12) the form

$$(3.14) \quad R_K \rightarrow \text{reg exp}(K^*), \quad u \mapsto u \cdot \mathbf{r}_{K^*}(u).$$

In angular coordinates the right-hand side is $e^{i\varphi} \cdot \mathbf{r}_{K^*}(e^{i\varphi}) = -\frac{e^{i\varphi}}{h_K(\varphi)}$ by (3.13). Thus the map (3.14) is locally at $e^{i\theta}$ of class C^k , as h_K at θ . Using (3.6),

$$\frac{\partial}{\partial \varphi} \left(-\frac{e^{i\varphi}}{h_K(\varphi)} \right) = \frac{x_K(e^{i\varphi})}{i h_K(\varphi)^2} \neq 0$$

holds, so the map (3.14) is locally at $e^{i\theta}$ a diffeomorphism. Since the inverse of (3.14) is continuous by a Theorem of Sz. Nagy [8], this proves that ∂K^* is locally at $\mathcal{C}_K(z) = e^{i\theta} \cdot \mathbf{r}_{K^*}(e^{i\theta})$ a C^k -submanifold of \mathbb{C} , see for example Section 3.1 of [1].

Let us prove that u_{K^*} is locally at $\mathcal{C}_K(z)$ a diffeomorphism. Since $x_K(e^{i\varphi}) = \nabla \mathbf{h}_K(e^{i\varphi})$ holds by (3.6), the reverse Gauss map x_K is locally at $e^{i\theta}$ of class C^{k-1} . The eigenvalue of $(dx_K)_{e^{i\theta}}$ is minus the radius of curvature of ∂K at $z = x_K(e^{i\theta})$ (see (3.8) and Lemma 3.1) which is assumed to be strictly positive. Therefore x_K is locally at $e^{i\theta}$ a C^{k-1} -diffeomorphism. Since $\mathcal{C}_K(z)/|\mathcal{C}_K(z)| = e^{i\theta}$ holds, the equation (3.11) shows that u_{K^*} is locally at $\mathcal{C}_K(z)$ a composition of C^{k-1} -diffeomorphisms and therefore u_{K^*} is itself locally at $\mathcal{C}_K(z)$ a C^{k-1} -diffeomorphism.

The claim follows by applying Lemma 3.2 and the preceding two paragraphs to K^* in place of K . More precisely, put $z^* := \mathcal{C}_K(z)$ and let $\theta^* \in \Xi_{K^*}^R$ be such that $z^* = x_{K^*}(e^{i\theta^*})$. Then Lemma 3.2 proves that h_{K^*} is locally at θ^* of class C^k and that the radius of curvature of ∂K^* is strictly positive at z^* . Replacing K, z, θ with K^*, z^*, θ^* , the preceding two paragraphs show that $\text{regexp}(K)$ is locally at $\mathcal{C}_{K^*}(z^*) = \mathcal{C}_{K^*}[\mathcal{C}_K(z)] = z$ a C^k -submanifold of \mathbb{C} and that u_K is locally at z a C^{k-1} -diffeomorphism. \square

We remark that the Gauss map u_K is a useful local chart for more general manifolds [39, 23] than the boundary of a convex body.

For completeness we discuss orientation of the reverse Gauss map of K . We assume that $0 \in \mathbb{R}^2$ is an interior point of K , so $h_K(\theta) < 0$ holds for all $\theta \in \mathbb{R}$. By the definition of $x_{K,\pm}$ and (3.2), the angle $\alpha_{K,\pm}(\theta)$ of the vector from $x_{K,\pm}(e^{i\theta})$ to the origin 0 is represented in the interval $[\theta - \frac{\pi}{2}, \theta + \frac{\pi}{2}]$ by the value

$$(3.15) \quad \alpha_{K,\pm}(\theta) = \theta \pm \arctan \left(\frac{\mathbf{h}'_K(e^{i\theta}; \pm i e^{i\theta})}{\mathbf{h}_K(e^{i\theta})} \right), \quad \theta \in \mathbb{R}.$$

Monotonicity of directional derivatives, $\mathbf{h}'_K(e^{i\theta}; i e^{i\theta}) \leq -\mathbf{h}'_K(e^{i\theta}; -i e^{i\theta})$, see for example Theorem 1.5.4 of [57], shows that

$$(3.16) \quad \alpha_{K,+}(\theta) - \alpha_{K,-}(\theta) \geq 0, \quad \theta \in \mathbb{R}.$$

Equality holds in (3.16) if and only if $x_{K,+}(\theta) = x_{K,-}(\theta)$, in which case we have $x_K(\theta) = x_{K,\pm}(\theta)$ and we define $\alpha_K(\theta) := \alpha_{K,\pm}(\theta)$. Assuming $\theta \in \Xi_K^{(2)} \subset \Xi_K$, the function h_K is twice differentiable at θ . Then equations (3.15), (3.3), and (3.7) prove

$$(3.17) \quad \alpha'_K(\theta) = \frac{h_K(\theta)}{h_K(\theta)^2 + h'_K(\theta)^2} [h_K(\theta) + h''_K(\theta)] \geq 0, \quad \theta \in \Xi_K^{(2)}.$$

Thereby $\alpha'_K(\theta) > 0$ holds if and only if $h_K(\theta) + h''_K(\theta) < 0$. In other words (3.8), the orientation of x_K is positive on open subsets of $\text{regn}(K)$ where x_K is a C^1 diffeomorphism.

4. DIFFERENTIAL GEOMETRY OF THE NUMERICAL RANGE

We study the smoothness of the boundary ∂W of the numerical range in terms of the smoothness of the ground state energy λ , including their differentiability orders. The analytic differential geometry of ∂W was studied earlier [26].

The support function \mathbf{h}_W of W at $u \in \mathbb{C}$ is the smallest eigenvalue of the hermitian matrix $\text{Re}(\bar{u}A)$. For unit vectors $e^{i\theta}$, as pointed out in (1.1), this means

$$h_W(\theta) = \mathbf{h}_W(e^{i\theta}) = \lambda(\theta), \quad \theta \in \mathbb{R}.$$

We will mostly work with λ in place of h_W or \mathbf{h}_W . We use angular coordinates θ and circular coordinate $\gamma(\theta) = e^{i\theta}$.

There is [53] an analytic curve of orthonormal bases of \mathbb{C}^d ,

$$(4.1) \quad |\psi_1(\theta)\rangle, \dots, |\psi_d(\theta)\rangle, \quad \theta \in \mathbb{R},$$

consisting of eigenvectors of $\operatorname{Re}(e^{-i\theta}A)$. The corresponding eigenvalues, also called *eigenfunctions* [41],

$$(4.2) \quad \lambda_k(\theta) := \langle \psi_k(\theta) | \operatorname{Re}(e^{-i\theta}A) \psi_k(\theta) \rangle, \quad k = 1, \dots, d,$$

are analytic. The 2π -periodic ground state energy

$$(4.3) \quad \lambda(\theta) = \min_{k=1, \dots, d} \lambda_k(\theta), \quad \theta \in \mathbb{R},$$

is continuous and piecewise analytic.

Piecewise analyticity of λ implies one-sided continuity properties summarized in Lemma 4.1. The easy proof is omitted, recall from (3.4) how $x_{W,\pm}$ depends on λ . For $n \in \mathbb{N}$ let the *left derivative* be defined by $\lambda^{\ell,(n)}(\theta) := -\lambda^{\ell,(n-1)'}(\theta; -1)$, and the *right derivative* by $\lambda^{r,(n)}(\theta) := \lambda^{r,(n-1)'}(\theta; +1)$, $\theta \in \mathbb{R}$, where $\lambda^{\ell,(0)} := \lambda^{r,(0)} := \lambda$. These derivatives exist throughout the real line and are one-sided continuous themselves.

Lemma 4.1. *For every $\theta \in \mathbb{R}$ there is $\epsilon > 0$ such that for all $n \in \mathbb{N} \cup \{0\}$ the maps $\lambda^{\ell,(n)}$ and $x_{W,-} \circ \gamma$ are continuous on $(\theta - \epsilon, \theta]$ and the maps $\lambda^{r,(n)}$ and $x_{W,+} \circ \gamma$ are continuous on $[\theta, \theta + \epsilon)$.*

We show that ∂W is a smooth envelope of supporting lines in the sense that the reverse Gauss map x_W is of class C^1 on its domain of regular normal vectors $\operatorname{regn}(W)$, where it is *a priori* only continuous [57]. The singular normal vectors form a finite set [16] corresponding to flat portions on the boundary of the numerical range. Therefore the set of angular coordinates $\Xi_W = \{\theta \in \mathbb{R} : e^{i\theta} \in \operatorname{regn}(W)\}$ is open. See Figure 2 for a commutative diagram.

Let the *maximal order* of λ at $\theta \in \mathbb{R}$ be the number $k \in \mathbb{N} \cup \{0\}$, if it exists, such that λ is k times continuously differentiable locally at θ , but not $k+1$ times. We use analogous definitions for other functions.

Lemma 4.2. *The ground state energy λ restricts to a C^2 -map on Ξ_W , which is analytic at $\theta \in \mathbb{R}$ if and only if there is an eigenfunction λ_k which equals λ in a neighborhood of θ . There exist at most finitely many points in $[0, 2\pi)$ at which λ is not analytic. The maximal order of λ at these points is even. For all $\theta \in \Xi_W$ the map x_W is analytic at $\gamma(\theta)$ if and only if λ is analytic at θ . Otherwise the maximal order of x_W at $\gamma(\theta)$ is the maximal order of λ at θ minus one.*

Proof: The 2π -periodic function λ is the pointwise minimum of finitely many analytic eigenfunctions λ_k by (4.3). Hence, λ is analytic on \mathbb{R} aside from finitely many exceptional angles $\theta \in [0, 2\pi)$ at which no single eigenfunction coincides with λ on a two-sided neighborhood of θ .

We show that the maximal order $m \in \mathbb{N} \cup \{0\}$ of λ at an exceptional angle θ is even. There exist $\epsilon > 0$ and $i_{\pm} \in \{1, \dots, d\}$ such that for $\varphi \in (\theta - \epsilon, \theta + \epsilon)$ we have

$$\lambda(\varphi) = \begin{cases} \lambda_{i_-}(\varphi), & \text{if } \varphi \in (\theta - \epsilon, \theta), \\ \lambda_{i_-}(\varphi) = \lambda_{i_+}(\varphi), & \text{if } \varphi = \theta, \\ \lambda_{i_+}(\varphi), & \text{if } \varphi \in (\theta, \theta + \epsilon). \end{cases}$$

Notice from Lemma 4.1 that if λ is k times differentiable at θ then it is of class C^k in a neighborhood of θ ; in particular $m \geq k$. Let the Taylor series of $\lambda_{i_+} - \lambda_{i_-}$ around

θ be given by

$$\lambda_{i_+} - \lambda_{i_-}(\varphi) = a_0 + a_1(\varphi - \theta) + \frac{a_2}{2}(\varphi - \theta)^2 + \frac{a_3}{6}(\varphi - \theta)^3 + \dots$$

We have $a_0 = 0$ because λ is continuous. If $m > 0$ then λ is differentiable at θ , so $a_1 = 0$. We show for $n \in \mathbb{N}$ that $a_{2n} = 0$, if $a_0 = \dots = a_{2n-1} = 0$. By contradiction, let $a_{2n} \neq 0$. Then

$$\lambda_{i_+}(\varphi) - \lambda_{i_-}(\varphi) = (\varphi - \theta)^{2n} \left[\frac{a_{2n}}{(2n)!} + \frac{a_{2n+1}}{(2n+1)!}(\varphi - \theta) + \dots \right]$$

is strictly positive (if $a_{2n} > 0$) or negative (if $a_{2n} < 0$) in a neighborhood of θ , which disagrees with the minimality of either λ_{i_-} on $(\theta - \epsilon, \theta)$ or λ_{i_+} on $(\theta, \theta + \epsilon)$. This proves that m is even. For $\theta \in \Xi_W$ we have $m \geq 2$ and $\Xi_W^{(2)} = \Xi_W$ follows.

It follows from $\Xi_W^{(2)} = \Xi_W$ that \mathbf{h}_W is C^2 on $\{\lambda u : \lambda > 0, u \in \text{regn}(W)\}$, as we pointed out above (3.7). Hence (3.6) shows that $x_W = (\nabla \mathbf{h}_W)|_{\text{regn}(W)}$ is a C^1 -map whose maximal order is one less than that of λ at corresponding points. Similarly, x_W inherits the analyticity from λ . \square

We show that the set of regular exposed points $\text{reg exp}(W)$ is a C^2 -submanifold of \mathbb{C} . This means that the Gauss map u_W is of class C^1 on $\text{reg exp}(W)$, where it is *a priori* only continuous [57]. With Corollary 4.7, this means that ∂W is a C^2 -submanifold of \mathbb{C} with the exception of corner points and non-exposed points. Again, see Figure 2 for a commutative diagram.

Let the *maximal order* of the boundary ∂W at $z \in \partial W$ be the number $k \in \mathbb{N}$, if it exists, such that ∂W is locally at z a C^k -submanifold of \mathbb{C} but not a C^{k+1} -submanifold.

Theorem 4.3. *The set $\text{reg exp}(W)$ is a C^2 -submanifold of \mathbb{C} and the Gauss map u_W restricts to a C^1 -diffeomorphism $\text{reg exp}(W) \rightarrow R_W$. Apart from at most finitely many exceptional points, $\text{reg exp}(W)$ is locally an analytic submanifold of \mathbb{C} . The maximal order is even at each exceptional point. Let $z \in \text{reg exp}(W)$ and $\theta \in \Xi_W^R$ such that $z = x_W(e^{i\theta})$. For all $k \geq 2$ the set $\text{reg exp}(W)$ is locally at z a C^k -submanifold of \mathbb{C} if and only if λ is locally at θ of class C^k . The set $\text{reg exp}(W)$ is locally at z an analytic submanifold of \mathbb{C} if and only if λ is analytic at θ .*

Proof: Lemma 4.2 proves that λ is of class C^2 on the open set Ξ_W . The radii of curvature of $\text{reg exp}(W)$ are finite by Lemma 3.1 and strictly positive by Theorem 2.4. Under these assumptions, Theorem 3.3 proves that $\text{reg exp}(W)$ is a C^2 -submanifold of \mathbb{C} , on which u_W defines a C^1 -diffeomorphism.

Using that u_W restricts to a C^1 -diffeomorphism on $\text{reg exp}(W)$ whose points have finite and strictly positive radii of curvature, Theorem 3.3 proves for all $k \geq 2$ that $\text{reg exp}(W)$ is locally at z a C^k -submanifold if and only if λ is locally at θ of class C^k . A modification of Theorem 3.3 proves that $\text{reg exp}(W)$ is locally at z an analytic submanifold if and only if λ is analytic at θ . Being piecewise analytic, λ has at most finitely many non-analytic points in $[0, 2\pi) \cap \Xi_W^R$. They correspond under $x_W \circ \gamma$ to the non-analytic points of $\text{reg exp}(W)$. The piecewise analyticity of λ shows also that the maximal order exists at every non-analytic point of λ . \square

We describe the set R_W of inner unit normal vectors at points of $\text{reg exp}(W)$, recall definitions from Figure 2. Let $\dim(W) = 2$ and let $N \in \mathbb{N} \cup \{0\}$ be the

number of facets of W . If $N \geq 1$ then we denote by

$$\alpha_0 < \cdots < \alpha_{N-1}$$

the angles in $[0, 2\pi)$ of the singular normal vectors $e^{i\alpha_0}, \dots, e^{i\alpha_{N-1}}$ of W , and we put $\alpha_N := \alpha_0 + 2\pi$. Let

$$O_i := \gamma[(\alpha_i, \alpha_{i+1})], \quad i = 0, \dots, N-1,$$

denote open arc segments of S^1 . We introduce labels for corner points. Let

$$S_A \subset [N] := \{0, \dots, N-1\}$$

include $i \in \{0, \dots, N-1\}$ if there exists $\theta \in (\alpha_i, \alpha_{i+1})$ such that $x_W(e^{i\theta})$ is a corner point of W . For $N = 0$ we observe that $R_W = S^1$.

Lemma 4.4. *Let $\dim(W) = 2$ and $N \geq 1$. The open arc segments and singular normal vectors $\bigcup_{i \in [N]} \{O_i, \{e^{i\alpha_i}\}\}$ form a partition of the unit circle S^1 . For every $i \in S_A$ the facets $F_W(e^{i\alpha_i})$ and $F_W(e^{i\alpha_{i+1}})$ intersect at a corner point $z(i)$ of W . The map $S_A \rightarrow W$, $i \mapsto z(i)$, defines a bijection from S_A to the set of corner points of W . The pre-image of $z(i)$ is $x_W^{-1}(\{z(i)\}) = O_i$, $i \in S_A$, and $R_W = \bigcup_{i \in [N] \setminus S_A} O_i$.*

Proof: The claimed partition of S^1 follows from the definition of the arc segments. If $i \in S_A$ then there is $\theta \in (\alpha_i, \alpha_{i+1})$ such that $z := x_W \circ \gamma(\theta)$ is a corner point of W . Table 1 shows that z is the intersection of two facets. Since the sequence $\alpha_0, \dots, \alpha_{N-1}$ is strictly increasing, we obtain $\{z\} = F_W(e^{i\alpha_i}) \cap F_W(e^{i\alpha_{i+1}})$. By definition of S_A , this construction exhausts all corner points of W , which proves the claimed bijection. The normal cones of W at $F_W(e^{i\alpha_j})$ are the rays spanned by $e^{i\alpha_j}$, $j = i, i+1$, both of which are faces of the normal cone of W at z , see for example [68]. This proves $x_W^{-1}(\{z\}) = O_i$. Since the open arcs O_i , $i \in S_A$, contain normal vectors at corner points and $\{e^{i\alpha_0}, \dots, e^{i\alpha_{N-1}}\}$ are singular normal vectors, the partition of S^1 shows $R_W \subset \bigcup_{i \in [N] \setminus S_A} O_i$. The definition of S_A shows the converse inclusion. \square

We distinguish a *counterclockwise* one-sided neighborhood of $z \in \partial W$, which extends from z in counterclockwise direction along ∂W , from a *clockwise* neighborhood.

Theorem 4.5 (Counterclockwise one-sided neighborhoods). *Let $z \in \text{reg ext}(W)$.*

- (1) *If $z \notin x_{W,+}(S^1)$ then z is a non-exposed point of W and $z = x_{W,-}(e^{i\alpha_{i+1}})$ holds for some $i \in [N] \setminus S_A$. The facet $F_W(e^{i\alpha_{i+1}})$ is a counterclockwise one-sided neighborhood of z in ∂W .*
- (2) *If $z = x_{W,+} \circ \gamma(\theta)$ for some $\theta \in \mathbb{R}$ then there exists $\epsilon > 0$ such that x_W restricts to an analytic diffeomorphism on $\gamma[(\theta, \theta + \epsilon)] \subset R_W$, and $x_{W,+}$ restricts to a homeomorphism on $\gamma\{[\theta, \theta + \epsilon)\}$. The image $x_{W,+} \circ \gamma\{[\theta, \theta + \epsilon)\}$ is a counterclockwise one-sided neighborhood of z in ∂W .*

Proof: (1) By definition of $x_{W,\pm}$, if $z \notin x_{W,+}(S^1)$ then z is a non-exposed point of W . Since every extreme point is in the image of either $x_{W,+}$ or $x_{W,-}$ there is $u \in S^1$ such that $z = x_{W,-}(u)$ holds. Since z is a non-exposed point, the vector u is a singular normal vector and (3.16) shows that the facet $F_W(u)$ extends counterclockwise from z . Since z is a non-exposed point, u cannot be the second vector of the pair $(e^{i\alpha_i}, e^{i\alpha_{i+1}})$ for any $i \in S_A$. Therefore $u = e^{i\alpha_{i+1}}$ for some $i \in [N] \setminus S_A$.

(2) Let $N \geq 1$. The 2π -periodicity of γ allows to choose $\theta \in [\alpha_0, \alpha_N)$. Notice that $\theta \notin [\alpha_i, \alpha_{i+1})$ for all $i \in S_A$ where $x_{W,+} \circ \gamma(\theta)$ is a corner point, if $\theta \in (\alpha_i, \alpha_{i+1})$

by Lemma 4.4 and if $\theta = \alpha_i$ by Lemma 4.1. So, Lemma 4.4 shows that there is $i \in [N] \setminus S_A$ such that $\theta \in [\alpha_i, \alpha_{i+1})$ and that $O_i = \gamma[(\alpha_i, \alpha_{i+1})]$ is included in R_W . Hence, Theorem 4.3 shows that x_W restricts to a C^1 -diffeomorphism on the open arc segment O_i . Lemma 4.2 points out that x_W has at most finitely many points of non-analyticity on O_i , so there is $\epsilon > 0$ such that x_W is an analytic diffeomorphism on $\gamma[(\theta, \theta + \epsilon)]$. This diffeomorphism extends to the continuous map $x_{W,+}|_{\gamma\{[\theta, \theta + \epsilon)\}}$ by Lemma 4.1, which is injective and therefore a homeomorphism (possibly for a smaller $\epsilon > 0$, allowing to use a compactness argument). The image $x_{W,+} \circ \gamma\{[\theta, \theta + \epsilon)\}$ is a counterclockwise one-sided neighborhood of z in ∂W by (3.17).

The proof of (2) for $N = 0$ is a shortened and simplified analogue of the proof for $N \geq 1$, because $R_W = S^1$ holds and $x_W : S^1 \rightarrow \partial W$ is a C^1 -diffeomorphism. \square

The clockwise analogue of Theorem 4.5 is as follows. We omit the proof.

Theorem 4.6 (Clockwise one-sided neighborhoods). *Let $z \in \text{reg exp}(W)$.*

- (1) *If $z \notin x_{W,-}(S^1)$ then z is a non-exposed point of W and $z = x_{W,+}(e^{i\alpha_i})$ holds for some $i \in [N] \setminus S_A$. The facet $F_W(e^{i\alpha_i})$ is a clockwise one-sided neighborhood of z in ∂W .*
- (2) *If $z = x_{W,-} \circ \gamma(\theta)$ for some $\theta \in \mathbb{R}$ then there exists $\epsilon > 0$ such that x_W restricts to an analytic diffeomorphism on $\gamma\{(\theta - \epsilon, \theta)\} \subset R_W$, and $x_{W,-}$ restricts to a homeomorphism on $\gamma\{(\theta - \epsilon, \theta]\}$. The image $x_{W,-} \circ \gamma\{(\theta - \epsilon, \theta]\}$ is a clockwise one-sided neighborhood of z in ∂W .*

A summary about the smoothness of ∂W can be useful.

Corollary 4.7. *Let $\dim(W) = 2$. The boundary ∂W with the (at most finitely many) corner points of W removed is a C^1 -submanifold M of \mathbb{C} . The maximal order of M is one at each of the (at most finitely many) non-exposed points of W . The remainder of M with non-exposed points removed is a C^2 -submanifold of \mathbb{C} , which is the union of relative interiors of facets of W with the set $\text{reg exp}(W)$ of regular exposed points.*

Proof: Since corner points of W_A are eigenvalues of A , see [19] and Section 2, there are at most finitely many of them. Theorem 2.2.4 of [57] shows that M is a C^1 -submanifold of \mathbb{C} (the proof of [57] can be applied locally at each regular boundary point of W). The numerical range W has at most finitely many non-exposed points z because each of them is an extreme point of a facet, of which there are at most finitely many [16]. Theorems 4.5 and 4.6 show that z is in the closure of $\text{reg exp}(W)$, more precisely in the closure of $x_W \circ \gamma(I)$ for some open interval $I \subset \Xi_W^R$, while Lemma 4.2 shows $\Xi_W^R \subset \Xi_W = \Xi_W^{(2)}$. Hence the ground state energy λ is a C^2 -map on I . Since λ is piecewise analytic, Lemma 3.1 proves that one of the one-sided radii of curvature $\rho_{\pm}(z)$ is finite. The other one-sided radius of curvature belongs to a facet of W and is infinite. Therefore the maximal order of ∂W locally at z is one. The remainder of M is a union of relative interiors of facets and $\text{reg exp}(W)$, see Section 2 and in particular Table 1. The differential geometry of $\text{reg exp}(W)$ is studied in Theorem 4.3. \square

5. ON THE CONTINUITY OF THE MAXENT MAP

We give a new proof that discontinuity points of the MaxEnt map $W_A \rightarrow \mathcal{M}_d$ constrained on expectation values of $\operatorname{Re}(A)$ and $\operatorname{Im}(A)$ correspond to crossings of class C^2 between a higher energy level and the ground state energy λ . The earlier proof uses stability of the state space \mathcal{M}_d and a result about lower semi-continuity of the inverse numerical range map. We also show that a weak form of this lower semi-continuity fails exactly at non-analytic points of ∂W of class C^2 .

We begin with continuity problems of the numerical range map. Let the unit sphere of \mathbb{C}^d be denoted by $S\mathbb{C}^d = \{|x\rangle \in \mathbb{C}^d : \langle x|x\rangle = 1\}$ and define the *numerical range map* of $A \in M_d$ by

$$f_A : S\mathbb{C}^d \rightarrow \mathbb{C}, \quad f_A(|x\rangle) = \langle x|Ax\rangle.$$

The image of f_A is the numerical range W_A . The (multi-valued) inverse

$$f_A^{-1} : W \rightarrow S\mathbb{C}^d$$

is called *strongly continuous* [18, 41] at $z \in W$, if for all $|x\rangle \in f_A^{-1}(z)$ the function f_A is open⁵ at $|x\rangle$. The map f_A^{-1} is called *weakly continuous* at $z \in W$, if there exists $|x\rangle \in f_A^{-1}(z)$ such that f_A is open at $|x\rangle$. We remark that f_A^{-1} to be strongly continuous at $z \in W$ is equivalently termed as f_A^{-1} to be *lower semi-continuous* at $z \in W$. The latter definition, see Section 6.1 of [8], goes back to Kuratowski and Bouligand.

It is known that strong continuity [18] of f_A^{-1} may fail only at points of the set of regular extreme points⁶ $\operatorname{reg ext}(W)$ of W and weak continuity [42] may fail only at points of the set of regular exposed points $\operatorname{reg exp}(W)$. See [45, 62] for further continuity studies of f_A^{-1} .

Continuity conditions of f_A^{-1} are known in terms of eigenvectors $|\psi_k(\theta)\rangle$, eigenfunctions $\lambda_k(\theta)$, $k = 1, \dots, d$, and ground state energy $\lambda(\theta)$ of the hermitian matrix $\operatorname{Re}(e^{-i\theta}A)$, introduced in equations (4.1), (4.2) and (4.3). Consider the analytic curves

$$(5.1) \quad z_k : \mathbb{R} \rightarrow \mathbb{C}, \quad \theta \mapsto f_A(|\psi_k(\theta)\rangle), \quad k = 1, \dots, d.$$

As was done in [41] we say that an eigenfunction λ_k *corresponds* to $z \in W$ at $\theta \in \mathbb{R}$, if $z = z_k(\theta)$ holds. The equation

$$(5.2) \quad z_k(\theta) = \gamma(\theta) \cdot [\lambda_k(\theta) + i\lambda'_k(\theta)], \quad \theta \in \mathbb{R},$$

follows by an easy calculation from Lemma 3.2 of [34]. We recall that $\gamma(\theta) = e^{i\theta}$.

We focus on extreme points of W . They can be written in the form $x_{W,\pm}[\gamma(\theta)]$ for some angle $\theta \in \mathbb{R}$. Recall from (3.1) that $e^{i\theta}$ is an inner unit normal vector of W at $x_{W,\pm}[\gamma(\theta)]$. Equation (3.4) shows

$$(5.3) \quad x_{W,\pm}[\gamma(\theta)] = \gamma(\theta) \cdot [\lambda(\theta) \pm i\lambda'(\theta; \pm 1)], \quad \theta \in \mathbb{R}.$$

By (5.2) and (5.3), for all $\theta \in \mathbb{R}$, an eigenfunction λ_k corresponds to $x_{W,\pm}[\gamma(\theta)]$ at θ if and only if

$$(5.4) \quad \lambda_k(\theta) = \lambda(\theta) \quad \text{and} \quad \lambda'_k(\theta) = \pm\lambda'(\theta; \pm 1),$$

that is λ_k agrees with the piecewise analytic λ to the first order on the right ($\pm = +$) or left ($\pm = -$) of θ . Since λ is piecewise analytic, the equation (5.4) is satisfied for

⁵This means that f_A maps neighborhoods of $|x\rangle$ in $S\mathbb{C}^d$ to neighborhoods of z in W .

⁶Section 2 explains the terminology of *round boundary points* used in [18, 41, 42].

each $\theta \in \mathbb{R}$ at least for one $k \in \{1, \dots, d\}$. This means that at least one eigenfunction corresponds to each extreme point at the angles of its inner normal vector(s).

Theorem 5.1 (Leake et al. [41]). *Let z be an extreme point of W and let $\theta \in \mathbb{R}$ be such that $z = x_{W,\pm}[\gamma(\theta)]$. Then f_A^{-1} is strongly continuous at z if and only if the eigenfunctions corresponding to z at θ are mutually equal as functions $\mathbb{R} \rightarrow \mathbb{R}$.*

Theorem 5.2 (Leake et al. [42]). *Let $z \in \text{reg ext}(W)$ and let $\theta \in \mathbb{R}$ be such that $z = x_{W,\pm}[\gamma(\theta)]$. Then f_A^{-1} is weakly continuous at z if and only if z lies in a facet of W or there exists an eigenfunction λ_k which equals λ in a neighborhood of θ .*

Lemma 4.2 and Theorem 4.3, combined with Theorem 5.2, prove the following.

Corollary 5.3. *Let $z \in \text{reg exp}(W)$. Then f_A^{-1} is weakly continuous at z if and only if ∂W is locally at z an analytic submanifold of \mathbb{C} .*

With Corollary 4.7 we get a second version of Corollary 5.3.

Corollary 5.4. *Let $z \in \partial W$. Then f_A^{-1} is weakly continuous at z if and only if ∂W is locally at z an analytic submanifold of \mathbb{C} , or z is a corner point or a non-exposed point of W .*

We turn to a maximum-entropy inference map. The *von Neumann entropy*, a measure of disorder of a state $\rho \in \mathcal{M}_d$, is defined by $S(\rho) := -\text{tr} \rho \log(\rho)$. Let $n \in \mathbb{N}$ and $\alpha : M_d^h \rightarrow \mathbb{R}^n$ be real linear. The *MaxEnt map* with respect to α is [30]

$$(5.5) \quad \alpha(\mathcal{M}_d) \rightarrow \mathcal{M}_d, \quad z \mapsto \text{argmax}\{S(\rho) : \rho \in \mathcal{M}_d, \alpha(\rho) = z\}.$$

The set $\alpha(\mathcal{M}_d)$ can represent expectation values, but also measurement probabilities or marginals of a composite system. In operator theory, $\alpha(\mathcal{M}_d)$ is known as the *joint algebraic numerical range* [48] or convex hull of the *joint numerical range*. The convex set $\alpha(\mathcal{M}_d)$ is isomorphic to the state space of an operator system [71]. For $n = 2$, $A \in M_d$, and

$$\alpha_A(B) := [\text{tr}(\text{Re}(A)B), \text{tr}(\text{Im}(A)B)] = \text{tr}(AB), \quad B \in M_d^h,$$

the set $\alpha_A(\mathcal{M}_d)$ is the numerical range W_A . Let

$$\rho_A^* : W_A \rightarrow \mathcal{M}_d$$

denote the MaxEnt map (5.5) resulting from $\alpha = \alpha_A$.

To analyze the continuity of ρ_A^* we first compute its values at extreme points. For any extreme point $z \in W_A$ and $\theta \in \mathbb{R}$ we consider the index set

$$K_A(z, \theta) := \{k \in \{1, \dots, d\} : z = z_k(\theta)\}$$

of eigenfunctions λ_k corresponding to z at θ , see (5.1). Let

$$(5.6) \quad X_A(z, \theta) := \text{span}\{|\psi_k(\theta)\rangle : k \in K_A(z, \theta)\}$$

and denote by $p_A(z, \theta)$ the projection onto $X_A(z, \theta)$.

We remark that the subspace $X_A(z, \theta)$ is the ground space of $\text{Re}(e^{-i\theta}A)$, if the supporting line of W with inner normal vector $e^{i\theta}$ meets W in a single point z . Indeed, we recall from Section 3 that the ground state energy λ is differentiable at θ and a comparison of power series coefficients, similar to Lemma 4.2, proves that all eigenfunctions λ_k which are minimal at θ also satisfy $\lambda'_k(\theta) = \lambda'(\theta)$. Now (5.4) proves that $X_A(z, \theta)$ is the ground space of $\text{Re}(e^{-i\theta}A)$. If $x_{W,+}(e^{i\theta}) \neq x_{W,-}(e^{i\theta})$ then the subspace $X_A(x_{W,\pm}(e^{i\theta}), \theta)$ is a proper subspace of the ground space of $\text{Re}(e^{-i\theta}A)$. Nevertheless this subspace defines the MaxEnt map at arbitrary extreme points.

Lemma 5.5. *Let $\theta \in \mathbb{R}$ and $z = x_{W,\pm}(\theta)$. Then*

$$f_A^{-1}(z) = S\mathbb{C}^d \cap X_A(z, \theta) \quad \text{and} \quad \rho_A^*(z) = p_A(z, \theta) / \text{tr } p_A(z, \theta).$$

Proof: Corollaries 2.4 and 2.5 of [62] prove that $f_A^{-1}(z)$ is the intersection of $S\mathbb{C}^d$ with the span of vectors $|\psi_k(\theta)\rangle$ whose indices $k \in \{1, \dots, d\}$ satisfy equation (5.4). These are the indices of eigenfunction λ_k corresponding to z at $\theta \in \mathbb{R}$, or equivalently $k \in K(z, \theta)$. By definition (5.6) of $X_A(z, \theta)$, this proves $f_A^{-1}(z) = S\mathbb{C}^d \cap X_A(z, \theta)$.

Since z is an extreme point of W , the fiber at z of the map $\mathcal{M}_d \rightarrow W$, $\rho \mapsto \text{tr}(\rho A)$ is a face $F(z)$ of \mathcal{M}_d . It is well-known, see for example [5, 2], that there exists a projection $p(z) \in M_d$ such that

$$F(z) = \{\rho \in \mathcal{M}_d : p(z)\rho p(z) = \rho\}.$$

It is easy to see that $\rho_A^*(z) = p(z) / \text{tr } p(z)$ holds. We complete the proof by showing $p(z) = p_A(z, \theta)$. For all $|x\rangle \in S\mathbb{C}^d$ we have $f_A(|x\rangle) = \text{tr}(|x\rangle\langle x|A)$ so we get

$$\begin{aligned} f_A^{-1}(z) &= \{|x\rangle \in S\mathbb{C}^d : |x\rangle\langle x| \in F(z)\} \\ &= \{|x\rangle \in S\mathbb{C}^d : p(z)|x\rangle = |x\rangle\} \\ &= S\mathbb{C}^d \cap \text{Image } p(z). \end{aligned}$$

This shows $X_A(z, \theta) = \text{Image } p(z)$ and hence $p_A(z, \theta) = p(z)$. □

To characterize the continuity of ρ_A^* we first study projections $p_A(z, \theta)$.

Lemma 5.6. *Let $z \in \text{reg ext}(W)$ and let $\theta \in \mathbb{R}$ be such that $z = x_{W,+}[\gamma(\theta)]$. Then there exists $\epsilon > 0$ such that $x_{W,+}$ restricts to a homeomorphism from $\gamma\{[\theta, \theta + \epsilon]\}$ to a counterclockwise one-sided neighborhood of z in ∂W (included in $\text{reg ext}(W)$). The map*

$$[\theta, \theta + \epsilon) \rightarrow 2^{\{1, \dots, d\}}, \quad \varphi \mapsto K_A(x_{W,+}[\gamma(\varphi)], \varphi),$$

is locally constant at θ if and only if

$$[\theta, \theta + \epsilon) \rightarrow M_d^h, \quad \varphi \mapsto p_A(x_{W,+}[\gamma(\varphi)], \varphi),$$

is continuous at θ if and only if the eigenfunctions corresponding to z at θ are mutually equal as functions $\mathbb{R} \rightarrow \mathbb{R}$. An analogue statement holds about $x_{W,-}$.

Proof: By Theorem 4.5(2) there is $\epsilon > 0$ such that $x_{W,+}$ restricts to a homeomorphism from $\gamma\{[\theta, \theta + \epsilon)\}$ to a counterclockwise one-sided neighborhood of z in ∂W . We denote the values of this homeomorphism by $z(\varphi) := x_{W,+}[\gamma(\varphi)]$ for $\varphi \in [\theta, \theta + \epsilon)$, so in particular $z = z(\theta)$. The equation (5.4) shows that $k \in K_A(z(\varphi), \varphi)$ holds if and only if

$$(5.7) \quad \lambda(\varphi) + i\lambda'(\varphi; 1) = \lambda_k(\varphi) + i\lambda'_k(\varphi).$$

Since λ is piecewise analytic, there is an index $\ell \in \{1, \dots, d\}$ and $\epsilon' > 0$ such that $\lambda(\varphi) = \lambda_\ell(\varphi)$ holds for $\varphi \in [\theta, \theta + \epsilon')$. Therefore, an eigenfunction λ_k satisfies (5.7) locally at θ in $[\theta, \theta + \epsilon)$ if and only if $\lambda_k = \lambda_\ell$. This proves that $K_A(z(\varphi), \varphi)$ is locally constant at θ in $[\theta, \theta + \epsilon)$ if and only if the eigenfunctions corresponding to z at θ are mutually equal as functions $\mathbb{R} \rightarrow \mathbb{R}$.

The equivalence of the continuity of $p_A(z(\varphi), \varphi)$ to the preceding statement follows from the continuity of the eigenvectors $|\psi_k(\varphi)\rangle$ in φ and the definition of p_A . Recall from (5.6) that $p_A(z(\varphi), \varphi)$ is the projection onto the subspace spanned by the eigenvectors $|\psi_k(\varphi)\rangle$ whose eigenfunctions λ_k correspond to $z(\varphi)$ and φ , that is

$z(\varphi) = z_k(\varphi)$, or $k \in K_A(z(\varphi), \varphi)$. \square

Like strong continuity of f_A^{-1} , continuity of ρ_A^* may fail only at points of $\text{reg ext}(W)$. This is shown in Section 6 of [54], using Donoghue's theorem, explained in Section 2, and topological ideas from Sections 4.2 and 4.3 of [69].

Theorem 5.7. *Let $z \in \text{reg ext}(W)$ and let $\theta \in \mathbb{R}$ be such that $z = x_{W,+}[\gamma(\theta)]$. Then ρ_A^* is continuous at z if and only if the eigenfunctions corresponding to z at θ are mutually equal as functions $\mathbb{R} \rightarrow \mathbb{R}$.*

Proof: Since z is a regular boundary point we have $\dim(W) = 2$, so ∂W is homeomorphic to S^1 . It is known that ρ_A^* is continuous at z if and only if $\rho_A^*|_{\partial W}$ is continuous at z , see Theorem 3.4 of [54]. Thus ρ_A^* is continuous at z if and only if $\rho_A^*|_U$ is continuous on a counterclockwise and a clockwise one-sided neighborhood U of z in ∂W . The two cases being similar, we study a counterclockwise neighborhood. Notice, from Section 2, that it is impossible to choose both one-sided neighborhoods as segments because z is a regular extreme point. One side yields the claimed continuity condition. The other side may yield the same or a trivial condition.

Let U be a counterclockwise one-sided neighborhood of z in ∂W . If U is a line segment then $\rho_A^*|_U$ is continuous at z because U contains a neighborhood of z which is a polytope [69]. Suppose that no counterclockwise one-sided neighborhood of z is a line segment. Then Theorem 4.5(1) shows that there is $\theta \in \mathbb{R}$ such that $z = x_{W,+} \circ \gamma(\theta)$. Theorem 4.5(2) shows that there exists $\epsilon > 0$ such that the homeomorphism

$$\zeta : [\theta, \theta + \epsilon) \rightarrow \text{reg ext}(W), \quad \varphi \mapsto x_{W,+}(e^{i\varphi}),$$

parametrizes a counterclockwise one-sided neighborhood of z in ∂W . The values of the MaxEnt map ρ_A^* at the image points of ζ are, by Lemma 5.5,

$$\rho_A^*[\zeta(\varphi)] = p_A(\zeta(\varphi), \varphi) / \text{tr } p_A(\zeta(\varphi), \varphi), \quad \varphi \in [\theta, \theta + \epsilon).$$

Since $\zeta(\theta) = z$ and since Lemma 5.6 shows that $\varphi \mapsto p_A(\zeta(\varphi), \varphi)$ is continuous at θ from the right, it follows that ρ_A^* is continuous at z from the counterclockwise direction if and only if the eigenfunctions corresponding to z at θ are mutually equal as functions $\mathbb{R} \rightarrow \mathbb{R}$. \square

Theorem 5.7 was proved earlier [70] using Theorem 5.1 as a black box and translating it to ρ_A^* using that the state space \mathcal{M}_d is *stable* [51, 58], which means that the mid-point map $(\rho, \sigma) \mapsto \frac{1}{2}(\rho + \sigma)$ is open.

We point out that Theorem 5.7 extends easily to inference maps [59, 60, 64] depending on a positive definite *prior state* $\rho \in \mathcal{M}_d$ which are defined by

$$\Psi_{A,\rho} : W_A \rightarrow \mathcal{M}_d, \quad z \mapsto \text{argmin}\{S(\sigma, \rho) : \sigma \in \mathcal{M}_d, \text{tr}(\sigma A) = z\}.$$

Here, the *Umegaki relative entropy* $S : \mathcal{M}_d \times \mathcal{M}_d \rightarrow [0, \infty]$ is an asymmetric distance. By definition, $S(\sigma, \rho) = \text{tr } \sigma(\log(\sigma) - \log(\rho))$ for positive definite ρ . Notice that $\Psi_{A, \mathbb{1}/d} = \rho_A^*$ holds, where $\mathbb{1}$ denotes the $d \times d$ identity matrix. It is easy to show that for extreme points z of W and $\theta \in \mathbb{R}$ such that $z = x_{W,+}[\gamma(\theta)]$ we have

$$\Psi_{A,\rho}(z) = \frac{p_A(z, \theta) e^{p_A(z, \theta) \log(\rho) p_A(z, \theta)}}{\text{tr } p_A(z, \theta) e^{p_A(z, \theta) \log(\rho) p_A(z, \theta)}}.$$

The proof of Theorem 5.7 readily applies to ρ_A^* replaced with $\Psi_{A,\rho}$, which shows that all inference maps $\Psi_{A,\rho}$ have the same points of discontinuity on W independent of the prior state ρ . This was proved by different methods in Theorem 7.1 of [70] for a much larger class of inference functions.

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